Research Program

Nuclear Energy and Waste Program

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Geological isolation of spent nuclear fuels and high-level radioactive waste is currently the preferred means of disposal for many countries worldwide. The role of ESD's Nuclear Waste Program (NWP) is to assist the U.S. Department of Energy, the United States, and other countries in achieving the safe disposal of high-level radioactive waste—by means of high-quality scientific analyses that encompass modeling, laboratory and field experiments, and technology development. Research within NWP focuses on flow and transport, as thermally driven hydrological, chemical, and mechanical coupled processes. Many of the studies within NWP relate to Yucca Mountain, the proposed site for the permanent storage of high-level nuclear waste in the USA; although NWP has also collaborated on nuclear-waste disposal issues with countries such as Japan, Finland, Switzerland, Spain, Sweden, and China.

The geologic repository program in the United States is at a point where the Department of Energy (DOE) is close to completing the license application for repository construction at Yucca Mountain to the Nuclear Regulatory Commission (scheduled for June 2008. The safe performance of a high-level nuclear waste repository hinges on the multiple-barrier concept—namely, that the natural system and the engineered system would each contribute significantly to prevent radionuclides from leaving the repository and entering the biosphere. The proposed repository at Yucca Mountain, consisting primarily of fractured volcanic tuffs that vary in degree of welding, will be located about 350 m below ground surface within a thick unsaturated zone (UZ) above the water table. Over the last decade, NWP's work at Yucca Mountain consists of site characterization studies aimed at understanding the barrier function of the UZ, through field testing in an underground facility, an 8 km long underground tunnel known as the Exploratory Studies Facility (ESF). Complex numerical models have also been developed to simulate and understand the relevant processes related to multiphase, nonisothermal flow and transport through the UZ. Some of the key questions addressed by NWP scientists include:

- How much water percolates through the UZ to the repository at Yucca Mountain?
- What fraction of the water flows in fractures and what fraction flows through the rock matrix blocks?
- How much of this water will seep into the emplacement drifts (tunnels)?
- How will the radionuclide migration from the repository to the water table be retarded?
- How will coupled TH (thermal-hydrological), THC (thermal-hydrological-chemical), and THM (thermal-hydro-logical-mechanical) processes affect flow and transport?

NWP scientists have also conducted studies as part of the Science and Technology (S&T) Program within the DOE Office of Civilian Radioactive Waste Management (OCRWM). Distinct from, but in parallel to, the licensing effort at Yucca Mountain, the role of the Science and Technology program is to advance technologies not previously considered, to identify new or substantially revised scientific methods or tools that would provide a better understanding of the repository environment.

LBNL ESD is the Lead for the Natural Barriers Thrust within the S&T Program. The goal for the Natural Barriers Thrust is to focus on research that would provide the essential scientific basis and demonstration of large contributions to repository performance by the unsaturated and saturated volcanic rocks at Yucca Mountain. The enhanced understanding of the different processes in the natural system would lead to reduction of uncertainty and obviate the need for overconservatism. NWP scientists are conducting studies pertaining to

- In-drift processes, integrating thermal-hydrologic-chemical-transport (THCM) models that simultaneously consider source term, corrosion, and the hydrological-chemical environment around waste package processes and conditions—and synthesize these complex processes into transparent, realistic, and defensible process models
- Near-drift processes, such as laboratory, field, and analogue studies to confirm the drift shadow concept, and the fact that it will lead to a large delay and sorption of radionuclides in the near-drift region
- Processes and conditions that will retard or mitigate flow and transport through the unsaturated and saturated volcanic rocks

FUNDING

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Geomechanical/Geochemical Modeling Studies Conducted with the International Cooperative Decovalex-THMC Project

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RESEARCH OBJECTIVES

DECOVALEX-THMC is an international cooperative project managed by SKI, the Swedish Nuclear Power Inspectorate. The general goal is to encourage collaborative research on modeling coupled thermal-hydrological-mechanical-chemical (THMC) processes in geologic formations in support of the performance assessment for underground storage of radioactive waste. One of the ongoing research tasks within this project, initiated in 2004 by the U.S. Department of Energy (DOE), addresses the long-term impact of geomechanical and geochemical processes on flow conditions near waste emplacement drifts. The objective of this task is to (a) develop new insights into such processes and (b) to provide valuable peer-review of the respective models and their prediction results.

Table 1. Research teams and simulators applied within DOE's DECOVALEX-THMC task.

Research Team	Simulator	Coupling	Mechanical/Chemical Model	Hydraulic and Transport Model
DOE/LBNL	TOUGH-FLAC	THM	Elastic, Elastoplastic, Viscoplastic	Discrete, single or dual continuum; multiphase liquid and gas flow
DOE/LBNL	ROCMAS	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
BGR/Center for Applied Geosciences (Germany)	Geosys/Rockflow	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
CAS, Chinese Academy of Sciences	FRT-THM	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
JAEA, Japan Atomic Energy Agency	THAMES	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
DOE/LBNL	TOUGHREACT	THC	Equilibrium and kinetic mineral-water-gas reactions HKF activity model	Discrete, single or dual continuum; multiphase liquid and gas flow; advection/ diffusion of total concentrations (sequential)
BGR/Center for Applied Geosciences (Germany)	Geosys/Rockflow with PHREEQC	THC	PHREEQC	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/diffusion of total concentrations (sequential)
JAEA, Japan Atomic Energy Agency	THAMES with Dtransu-3D-EL and PHREEQC	THMC	PHREEQC	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/ diffusion of total concentrations (sequential)

APPROACH

The four research teams (from China, Germany, Japan, and USA) participating in DOE's task within the DECOVALEX-THMC project were asked to conduct predictive analysis of the long-term coupled processes in generic repositories with simplified conditions and geometry. Participating research teams model the THMC processes in the fractured rock close to a representative emplacement drift as a function of time, predict long-term changes in hydrological properties, and evaluate the impact on near-field flow and transport processes. Two generic repositories situated in different host rock types and featuring different emplacement conditions are analyzed for comparison. One is a simplified repository model of the United States' Yucca Mountain site, a deep unsaturated volcanic rock formation with emplacement in open gas-filled drifts. The second repository model is "located" in saturated crystalline rock, with emplacement drifts backfilled using a low-permeability buffer material such as bentonite (a concept considered in many European countries and in Japan).

ACCOMPLISHMENTS

As shown in Table 1, the research teams use different codes with different model approaches and characteristics. Since all teams simulate the same task configuration, research results from the participating teams can be directly compared. To date, good progress has been made in both model development and application. Comparison of geomechanical results indicates good overall agreement with respect to temperatures, stresses, and various hydrological parameters, despite the fact that different model approaches were used. Geochemical models show good quantitative agreement regarding aqueous species concentrations, while some differences with respect to mineral alterations still need to be worked out.

SIGNIFICANCE OF FINDINGS

The collaborative research conducted by international teams helps to develop a broader understanding of the complex THMC processes occurring near geologic repositories for radioactive waste. Good agreement between simulation results obtained with different model approaches provides enhanced confidence in their predictive capabilities when applied, for example, to the proposed Yucca Mountain repository.

RELATED PUBLICATIONS

Birkholzer, J., D. Barr, J. Rutqvist, and E.L. Sonnenthal, Motivation, description, and summary status of geomechanical and geochemical modeling studies in Task D of the International DECOVALEX Project. Proceedings, Geoproc 2006, China, May 2006.

Rutqvist, J., J. Birkholzer, M. Chijimatsu, O. Kolditz, Q. Liu, Y. Oda, W. Wang, and C. Zhang, Comparative simulation study on coupled THM processes near back-filled and open-drift nuclear waste repositories in Task D of the International DECOVALEX Project. Proceedings Geoproc 2006, China, May 2006.

Xie, M., E.L. Sonnenthal, W. Wang, O. Kolditz, J. Birkholzer, Y. Oda, and M. Chijimatsu, Geochemical predictions for a hypothetic repository located in saturated crystalline rock—Comparative evaluation of two different research teams. Proceedings Geoproc 2006, China, May 2006.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of the Chief Scientist, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Continuous-Time Random-Walk Analysis of Dual-Permeability Fractured Media

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RESEARCH OBJECTIVES

Reliable prediction of fluid and solute movement in fractured porous formations is of paramount importance in many practical applications. Fracture networks and the surrounding porous (and permeable) matrix are not hydraulically independent domains—they interact by exchanging solutes at their interface. Solute particles traveling on fast flow paths in the fractures can be retarded by solute exchange with the porous matrix, a diffusive or advective process depending on matrix properties. These retardation effects are extremely difficult to model in a classical transport framework. The objective of this research is to apply the continuous-time random-walk (CTRW) transport theory to the analysis of dual-permeability fractured media, to characterize transport by means of probabilistic distributions of the solute retention times.

APPROACH

In the CTRW approach, the interaction between the fractured and porous rock domains is modeled by a transition time probability distribution function (pdf), which characterizes the retention time inside the fractured medium. In our research, this approach is validated numerically through the analysis of discrete numerical solutions of tracer transport in idealized dual permeability fractured media. A numerical inversion procedure identifies the transition time pdf from the analysis of the BTCs.

ACCOMPLISHMENTS

We applied the CTRW analysis to a series of synthetic breakthrough curves (BTC) obtained by means of a standard finite element code, on a finely gridded 2-D geometry consisting of a regular arrangement of fractures (oriented at a 45º angle with respect to the direction of the mean flow) in a permeable porous domain (see Figure 1). By changing matrix permeability over a wide range (from representing rather permeable sandstone on one end of the spectrum to almost impermeable granites or shales on the other), we have considered various fracture-to-matrix permeability contrasts, which reflect typical values of densely fractured geological formations.

SIGNIFICANCE OF FINDINGS

Our results indicate that a CTRW analysis can completely characterize transport in dual-permeability fractured media by means of a probabilistic distribution function (pdf) of solute retention times. The pdf can be obtained from an analysis of the macroscopic (experimental) BTCs and contains all the necessary information for predicting the solute behavior at different times and sections. In the CTRW model, the transport velocity can be estimated from the composite porosity of the dual permeability medium. Furthermore, the classical dispersivity parameter, an essential component of any advection-dispersion based model, does not scale with the distance of the observation, but rather stays constant and relatively small. These findings indicate the CTRW method is an important and valuable alternative to more complex model approaches for fractured porous formations, such as discrete models or dual-permeability formulations.

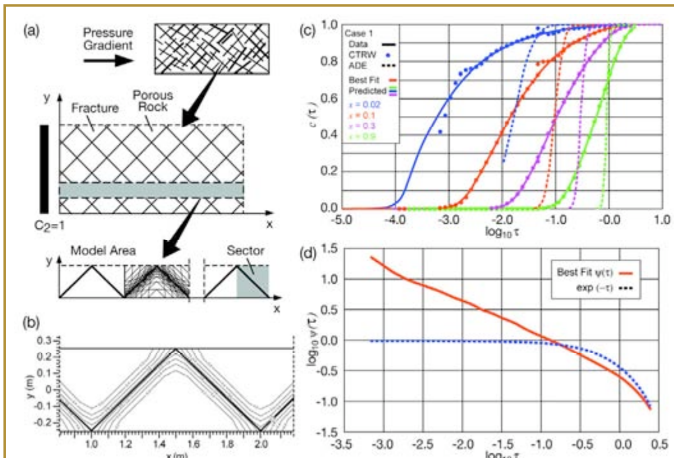

Figure 1. (a) Fractured domain under study (b) Discrete finite-element solute-transport simulations for a permeability contrast of approximately 12,000. (c) Breakthrough curves at four different sections. Discrete simulations are solid lines; CTRW predictions are circles; advection dispersion equation (ADE) predictions are dashed lines. (d) Probabilistic distribution of the solute residence times from CTRW analysis (red line), and comparison with the decaying exponential distribution (ADE model).

RELATED PUBLICATIONS

Cortis, A., Peclet-dependent memory kernels for transport in heterogeneous media. Phys Rev. E, 2007 (submitted).

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of the Chief Scientist, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Heterogeneous Seepage at the Nopal I Uranium Mine, Chihuahua, Mexico

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RESEARCH OBJECTIVES

The primary objective of this analogue study is to evaluate flow and transport processes of relevance to the proposed Yucca Mountain repository. Seepage data obtained from this study will be used to constrain flow and transport models being developed for the Nopal I system.

APPROACH

A water collection system, consisting of 240 separate 30 cm × 30 cm compartments that are each connected to a 125 mL bottle, was installed in April 2005 within the +00 m adit of the Nopal I mine, to collect water that had infiltrated from the +10 m level and seeped into the adit. This system was upgraded in November 2005, when instrumentation was added to six collector sites to measure seepage rates continuously. An automated weather station was installed at the site in March 2006 to permit correlation of local precipitation events with seepage.

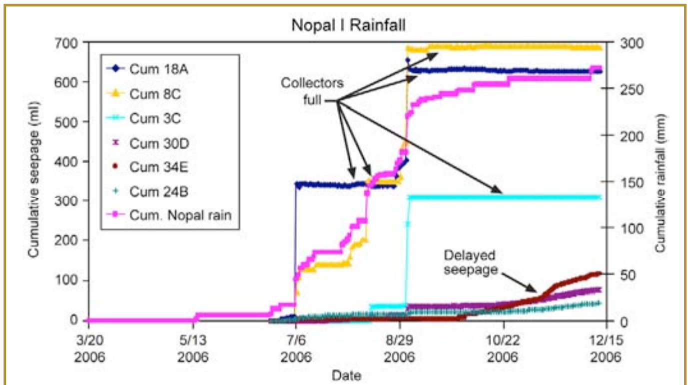

Figure 1. Cumulative rainfall and seepage amounts for instrumented collectors from Nopal I +00 m adit.

ACCOMPLISHMENTS

Rainfall in central Chihuahua is seasonal, with most precipitation occurring during the summer monsoon period. Initial modeling of infiltration and seepage through a series of planar, vertical fractures was conducted to evaluate flow transit times and seepage rates (Ghezzehei et al., 2006). Using a range of fracture apertures and frequencies, and assuming no fracture-matrix interaction, infiltration through the 8 m high vertical fracture system and seepage into the adit was predicted to occur within 24 hours after a 6-hour rainfall event.

Monitoring of seepage within the adit between April 2005 and December 2006 indicates that seepage is highly heterogeneous in both time and space. Within the back adit area, there are a few zones where large volumes of water have been collected. These large volume seepage events (Figure 1) are linked to fast flow path fractures (<4 h transit times) and are associated with heavy rainfall (>25 mm). In most locations, however, there is a significant (1–6 month) time lag between major precipitation events and seepage within the adit, with longer water residence times observed for the front adit area.

SIGNIFICANCE OF FINDINGS

The wide variability in the location, timing, and amount of seepage occurring within the Nopal I adit suggests that a number of fast-flow fracture pathways are active immediately after large rainfall events. Flow focusing along these pathways may explain the heterogeneous seepage distribution. However, delayed seepage observed in many locations within the adit indicate that even a relatively thin (8 m) rock mass can exert a noticeable damping effect on infiltration, and that flow and transport models must incorporate fracture flow heterogeneity. The initial results of this work are consistent with the fast-flow-path model postulated for Yucca Mountain.

RELATED PUBLICATIONS

Ghezzehei, T.A., P.F. Dobson, J.A. Rodriguez, and P.J. Cook, Infiltration and seepage through fractured welded tuff. 2006 International High Level Radioactive Waste Management Conference, April 30–May 4, 2006, Las Vegas, NV, American Nuclear Society, La Grange Park, IL, pp. 105–110, 2006.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of the Chief Scientist, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231. We thank the Instituto de Ecologia, A.C. and the Universidad Autónoma de Chihuahua for their assistance.

Evaluation of Uncertainties due to Hydrogeological Modeling and Groundwater Flow Analysis: Strategy for Characterizing a New Site

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RESEARCH OBJECTIVES

It is quite challenging to build a reliable model for simulating groundwater flow in a large body of rock mass, particularly when the rock is fractured. Large-scale groundwater flow models are typically calibrated to the steady-state pressure head data. However, steady-state head data alone are not sufficient for building a reliable predictive model. The overall objective of this project is to develop methodologies for reducing the uncertainty and increasing the reliability of such a model. In the present work, we develop a strategy for characterizing a new site where a minimal number of wells are available.

APPROACH

We begin with a 9 km × 9 km × 2 km thick effective continuum model of the fractured rock of the Tono, Japan, area developed from regional geographic, geologic, geophysical, and surface and subsurface hydrological data. The model is calibrated simultaneously to data from 17 wells: steady-state head profiles in 11 wells, 21 pressure transients from 8 wells, and steady-state temperature profiles in 11 wells, which constrain the porosity and permeability of the granitic rock, overlying sediments, and a major subvertical fault that bisects the model. Also so constrained are the amount of surface infiltration that recharges the deep groundwater flow system and the lateral boundary conditions of the model. The resulting model is considered the best model possible of the Tono region, since it utilizes the full set of available data.

Next, we consider data from various subsets of these 17 wells and compare performance measures obtained from the resulting models to those of the best model, to investigate how many wells to use and how to optimally locate wells for a preliminary site characterization. Additionally, some of the key assumptions regarding model heterogeneity and boundary conditions are examined to assess the impact they have on recommended well locations.

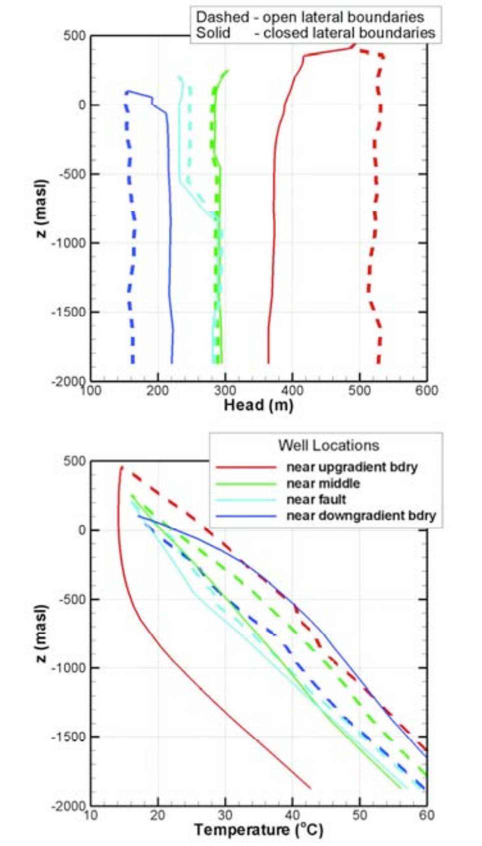

Figure 1. Head (top) and temperature (bottom) profiles at four hypothetical well locations (different colors), for closed and open lateral boundaries (different line styles). Profiles from wells located near the boundaries are useful for characterizing lateral boundary conditions.

ACCOMPLISHMENTS

We find that, for the most part, our understanding of the regional groundwater flow and advective tracer transport does not improve significantly as more and more wells are used for site characterization. This is because these measures are controlled by surface topography, surface and lateral boundary conditions, and permeability and porosity distributions, and the present property distributions have short correlations, hence using one well for site characterization provides as much information about material properties as using many wells does.

On the other hand, observing head profiles in more wells increases the probability that large-scale features that do impact groundwater flow (such as a fault) can be identified. An additional caveat is that if the permeability distribution has long-range correlations, then a small number of wells are not as likely to provide a representative sample of rock properties, nor a true picture of the regional groundwater flow.

SIGNIFICANCE OF FINDINGS

Lateral boundary conditions have a large impact on all aspects of flow and transport. If existing studies of topography and regional groundwater flow do not provide this information, wells should be located near the presumed upgradient and downgradient boundaries of the site, and head and temperature profiles should be examined for the characteristics of closed and open groundwater flow systems.

RELATED PUBLICATION

Karasaki, K., J. Apps, C. Doughty, H. Gwatney, C.T. Onishi, R.C. Trautz, and C.F. Tsang, Feature Detection, Characterization and Confirmation Methodology—Final Report. NUMO-LBNL Collaborative Research Project Report, March 2007.

ACKNOWLEDGMENTS

This work is supported by the Nuclear Waste Management Organization of Japan (NUMO) and the Japan Atomic Energy Agency (JAEA) through a bi-national agreement between JAEA and the U.S. Department of Energy (DOE), and conducted at the Ernest Orlando Lawrence Berkeley National Laboratory under DOE Contract No. DE-AC02-05CH11123.

Berkeley Lab

Analysis of Flowing Fluid-Electric-Conductivity Logs under Nonideal Conditions

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RESEARCH OBJECTIVES

In the study of flow and transport in the subsurface, knowledge of flow zones and their hydraulic properties is essential. Coring and geophysical methods in boreholes drilled deep into the rock may be able to identify the fractures themselves, but they are unlikely to provide information on fracture flow properties. Straddle-packer pump-testing yields fracture flow properties, but is very time-consuming. Flow-logging techniques are an attractive alternative—they are sensitive to fracture flow and are efficient to deploy in the field.

The flowing fluid-electric-conductivity (FFEC) logging method provides information on the depths, salinities, transmissivities, and pressure heads of individual conductive features intercepted by a borehole, without the need of specialized probes. The method has been successfully applied to deep boreholes in granitic formations. This summary presents the application of the method to two zones in a 1,000 m borehole in sedimentary rock at Horonobe, Japan. The data sets involve a number of complications, such as variable well diameter, free water table decline in the well, periods of time with unknown pumping rate, and effects of drilling mud. Our objective is to determine whether the method is robust enough to use under these nonideal conditions.

APPROACH

The FFEC logging method involves the replacement of wellbore water by de-ionized water, followed by pumping at a constant rate, during which a series of fluid electric conductivity logs are taken. The logs can be analyzed to identify depth locations of inflow, and evaluate inflow rate and electric conductivity (salinity) of the fluid at each inflow point. When the method is repeated with two or more pumping rates, a combined analysis of the multi-rate data allows an efficient means of also determining transmissivity values of all inflow points, as well as their inherent (so-called far-field) pressure heads.

For each of the two zones logged in the 1,000 m wellbore, three sets of logs were collected using different pumping rates, each set measured over a period of about one day (Figure 1). To analyze the data, we apply various techniques that have been developed for analyzing FFEC logs: direct-fitting, mass-integral, and the multi-rate method mentioned above.

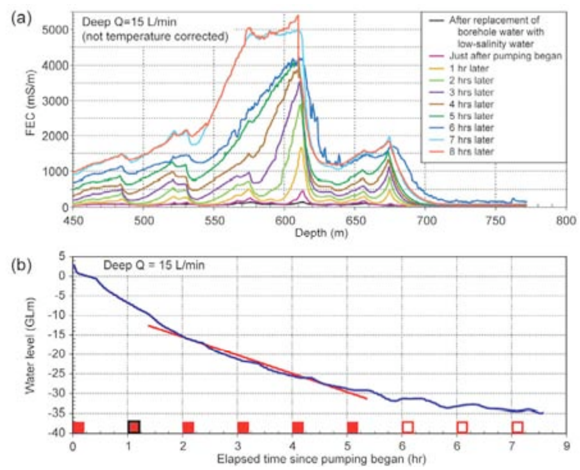

Figure 1. Sample of FFEC data, illustrating some of the complications: (a) Set of FFEC logs for a deep-zone test. Logs obtained 6, 7, and 8 hours after pumping began are not consistent with other logs, probably owing to slime from drilling mud adhering to the probe; (b) Water-level data during logging. Red boxes identify times at which logs were collected; open boxes indicate a problem with the FFEC log; the black-outlined box was used as initial conditions for model. A period of high, unknown pumping rate occurred early on, causing a sudden water-level decline. Thereafter, water-level declined steadily, but at a decreasing rate. Only logs collected while the decline is approximately linear (red line) are analyzed.

ACCOMPLISHMENTS

In spite of complications associated with the tests, analysis of the data is able to identify 44 hydraulically conducting fractures distributed over the depth interval 150–775 m below ground surface with resolution of about 0.2 m. The salinities (in FEC), and transmissivities and pressure heads (in dimensionless form) of these 44 features are obtained and found to vary significantly among one another. These results are compared with data from eight packer tests with packer intervals of 10–80 m, which were conducted in this borehole over the same depth interval. They are found to be consistent with these independent packer-test data, thus demonstrating the robustness of the FFEC logging method under nonideal conditions.

SIGNIFICANCE OF FINDINGS

FFEC logging provides an efficient, affordable means of characterizing the hydraulically conductive features intersecting a borehole, with high vertical resolution and without the need of specialized probes. Such information is valuable for characterization of regional groundwater flow, design of nuclear waste storage facilities, remediation of subsurface contamination, and a host of other problems. Moreover, it can be very useful in conjunction with other subsurface site-characterization activities, such as providing high-resolution monitoring during a tracer test, or providing ground truth at boreholes for crosshole geophysical imaging methods.

RELATED PUBLICATIONS

Doughty, C., C.-F. Tsang, K. Hatanaka, S. Yabuuchi and H. Kurikami, Application of direct-fitting, mass-integral, and multi-rate methods to analysis of flowing fluid electric conductivity logs from Horonobe, Japan. LBNL-63307. Water Resour. Res. (in press), July 2007.

ACKNOWLEDGMENTS

This work is supported by the Nuclear Waste Management Organization of Japan (NUMO) and the Japan Atomic Energy Agency (JAEA), through a bi-national agreement between JAEA and the U.S. Department of Energy (DOE), and conducted at Berkeley Lab under DOE Contract No. DE-AC02-05CH1123.

Climatic Forecasting of Net Infiltration at Yucca Mountain Using Analogue Meteorological Data

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RESEARCH OBJECTIVES

The objective is to develop a semi-empirical model and forecast average net infiltration rates, using the limited meteorological data from analogue meteorological stations, for interglacial (present-day), and future monsoon, glacial transition, and glacial climates over the Yucca Mountain region.

APPROACH AND METHODS

Net infiltration, aridity, and precipitation-effectiveness (P-E) indices were calculated using a modified Budyko's water-balance model, with reference surface potential evapotranspiration determined from the radiation-based Penman formula. The computed net infiltration rates were corroborated by comparing them with the empirically and numerically determined groundwater recharge and percolation rates through the unsaturated zone from published data.

ACCOMPLISHMENTS

Net infiltration rates are forecasted to generally increase from the present-day climate to monsoon climate, to glacial transition (intermediate) climate, and then to the glacial climate, following a power law relationship between net infiltration and precipitation. The forecasting results indicate the overlap between the ranges of net infiltration for different climates (Figure 1). The calculated net infiltration rates have yielded a good match with other field and modeling study results pertaining to groundwater recharge and percolation flux through the unsaturated zone at Yucca Mountain. This comparison indicates the robustness of the simple water-balance approach used in this study.

SIGNIFICANCE OF FINDINGS

Computed present-day and potential future net infiltration can be used as a hydrologic parameter to assess the rate of deep percolation, groundwater recharge, radionuclide transport, and seepage into tunnels—all of which are, in turn, useful parameters for the performance assessment of the proposed nuclear waste repository at Yucca Mountain, Nevada.

RELATED PUBLICATION

Faybishenko, B., Climatic forecasting of net infiltration at Yucca Mountain using analogue meteorological data. Vadose Zone Journal, 6, 77–92, 2007.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

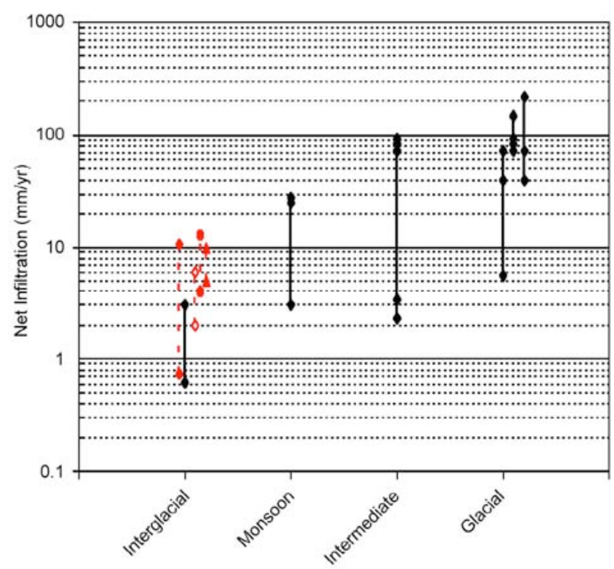

Figure 1. Climatic ranking of ranges of forecast net infiltration for different climates. Red dashed lines show the ranges of the percolation flux from calculations using a Cl mass-balance model (solid diamonds), calcite mass model (open diamonds), temperature data (closed circles), and experts' evaluation (solid triangles).

A Modeling Study on Natural Convection in Emplacement Drifts and Its Impact on Drift Seepage

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RESEARCH OBJECTIVES

The decay heat outputs of the radioactive waste potentially to be emplaced at Yucca Mountain will strongly affect the thermal-hydrological (TH) conditions in and near the geologic repository. This decay heat elevates drift temperatures above ambient conditions. Pore formation water in the near-field rock mass evaporates into the open air spaces of the drift and is transported by natural convection processes from the hot drift center to the cool drift end (where no waste is emplaced) and condenses. Our goal is to better understand this reduction of moisture content in the near-drift fractured rock and its role in the potential reduction of seepage into the drift.

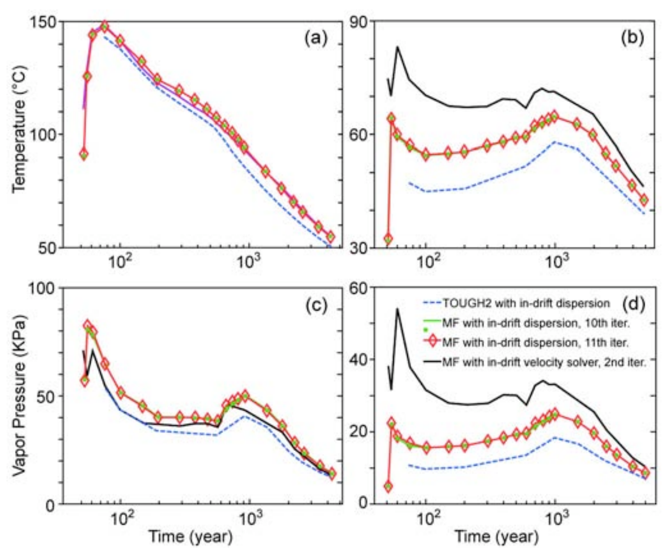

Figure 1. Drift wall temperature evolution at the hottest (a) and coldest (b) drift segments; and vapor-pressure evolution at the hottest (c) and coldest (d) drift segments.

APPROACH

A multiscale seepage modeling procedure was developed that accounts for transport processes in and between the fractured rock mass and the open air drift, two distinct domains. To fully account for 3-D effects, a first model (MF-T2) operates on a scale that encompasses the entire drift plus surrounding rock units. In MF-T2, the flow and transport processes in the rock mass are simulated with the multiphase, multicomponent simulator TOUGH2, and the in-drift heat and moisture flows are simulated with MULTIFLUX (MF), a lumped-parameter CFD (Computational Fluid Dynamics) code (Danko et al., 2007). MF provides an efficient iterative coupling technique for matching the mass and heat transfer between the rock mass and the drift. In addition, explicit modeling of the impact of in-drift moisture transport on seepage is being conducted with a separate high-resolution seepage model, with model inputs (in-drift temperature and relative humidity) provided by the full drift-scale MF-T2 model.

ACCOMPLISHMENTS

The new solution procedure has been applied to evaluate the heat-driven flow and transport processes in a representative emplacement drift at Yucca Mountain, embedded in a monolithic, three-dimensional rock mass. Two alternative approaches were tested to simulate in-drift natural convection: (1) a lumped-parameter CFD dispersion model and (2) a model explicitly simulating the air velocity distribution. Several iterations were completed, refreshing the MF results against TOUGH2 runs, with both solution procedures showing excellent convergence (Figure 1). Also, alternative results from a simplified in-drift model within TOUGH2 are shown (Birkholzer et al., 2006). High-resolution seepage model development is ongoing, with preliminary results indicating that strong natural convection processes can significantly reduce the near-field fracture moisture content, thereby reducing the seepage potential.

SIGNIFICANCE OF FINDINGS

The difficult task of coupling CFD models with porous media models, to understand moisture reduction in the near drift, is undertaken with a unique and efficient approach. Initial results from the coupled MF-T2 solution procedure show good convergence between the two domains for a full drift-scale representation. The ongoing efforts of applying results from these simulations into a high-resolution seepage model will allow for a better understanding of seepage reduction due to natural convection processes, thereby further characterizing potentially beneficial repository behavior.

RELATED PUBLICATIONS

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Danko, G., D. Bahrami, and J.T. Birkholzer, The effect of unheated sections on moisture transport in the emplacement drift. Nuclear Technology (in press), 2007.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of the Chief Scientist, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Examining the Drift Shadow in Nature

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RESEARCH OBJECTIVES

The drift shadow is a region in the unsaturated zone beneath an underground opening (such as a cave or mined tunnel) that is partially sheltered from downward-percolating water, because the capillarity is not strong enough to draw water into the rock immediately below the drift. Modeling studies of the drift shadow suggest that transport in this region is controlled by diffusive rather than by advective processes. The drift shadow has not yet been observed in nature. Our research objective is to demonstrate the presence (or absence) of the drift shadow at a field location and compare our measurements to predictions.

APPROACH

To identify a drift shadow, we must find an appropriate field site where a drift shadow might be observed, obtain core samples from locations at different depths around the opening, and make measurements of water potential and water content that would indicate the presence or absence of the drift shadow. In addition, we would like to impose a water flux over a drift and observe its flow behavior and possible drift shadow formation. We must also compare our field results with modeling results of a detailed site-specific model to gain confidence in modeling studies of the drift shadow.

ACCOMPLISHMENTS

We have performed extensive modeling to understand the theoretical definition and extent of the drift shadow for various sets of conditions. Based on our modeling, we selected and are investigating the presence of the drift shadow in the East Bay Regional Parks District Hazel-Atlas Mine, a former sand mine in Northern California that is now operated as a museum. Our study location, not currently in the museum, contains a drift-over-drift configuration. We have retrieved core from core holes fanning the two drifts, x-ray-scanned them looking for density changes, and measured gravimetric moisture content of subsamples of the core. We have performed ground-penetrating radar studies using the core holes to look for saturation changes indicating the presence of a drift shadow and are constructing an active test to impose water flow around the lower drift.

SIGNIFICANCE OF FINDINGS

Demonstrating the presence of a drift shadow will provide another line of evidence to build confidence in the theory of flow and transport in unsaturated media and its numerical extension. In addition, it will allow the consideration of significantly reduced transport from waste emplacement drifts at the proposed high-level nuclear waste repository at Yucca Mountain, Nevada, in which waste packages are expected to be placed in near-horizontal drifts in the unsaturated zone.

RELATED PUBLICATIONS

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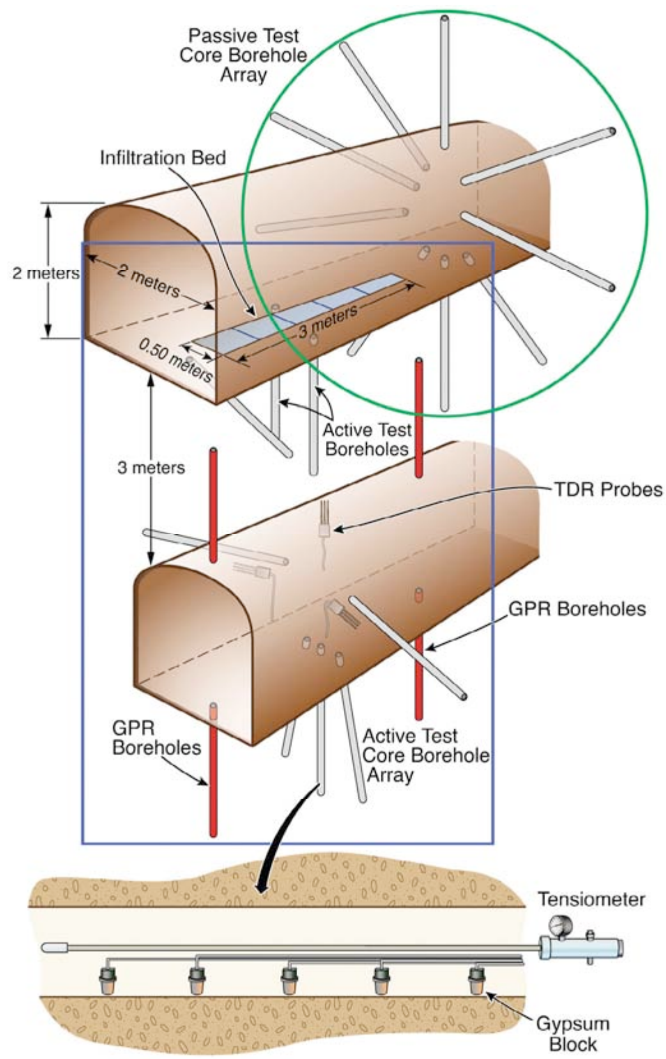

Figure 1. Schematic of boreholes and test setup. Green circle is the core analysis and GPR, blue rectangle is the active test, red lines are the continued GPR measurements.

ACKNOWLEDGEMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of the Chief Scientist, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Sensitivity Analysis for Joint Inversion of Ground-Penetrating Radar and Thermal-Hydrological Data from a Large-Scale Underground Heater Test

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RESEARCH OBJECTIVES

To develop site-specific hydrological models, the joint analysis of hydrological and geophysical data has the potential to significantly improve the characterization of the subsurface, and thus increase the reliability of model predictions. The merit of any given data type depends on its usefulness in providing quantitative information about flow and transport properties (at a reasonable resolution). Since geophysical data offer valuable information on the subsurface structure, developing methods for integrating such data with hydrological data has the potential to significantly advance site characterization in complex, heterogeneous systems.

The objective of this research is to develop a joint inversion approach so that it can be applied to increasingly complex thermal-hydrological processes. These processes include the transport of water, water vapor, air and heat in fractured porous media, the transitions between the liquid and gaseous phases, and vapor-pressure lowering effects as a result of capillary pressure increases.

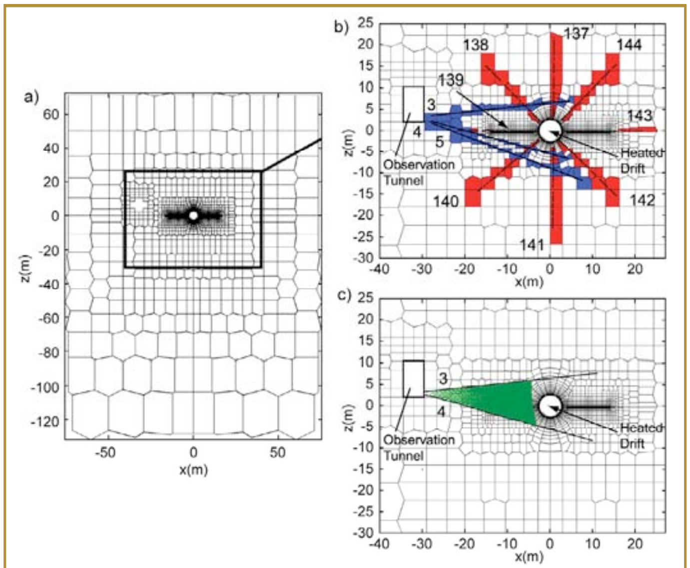

Figure 1. Thermal-hydrological model and measurement locations: (a) model grid; (b) locations of water content (measured by neutron probes) and temperature measurements (indicated by blue- and red-shaded gridblocks, respectively); and (c) locations for ground-penetrating radar data used for inversion (green lines connect transmitting and receiving antennas).

APPROACH

The approach integrates the coupled simulation of thermal-hydrological and geophysical data—ground-penetrating radar (GPR) data—within the iTOUGH2 optimization framework to estimate (1) thermal-hydrological parameters (such as permeability, porosity, thermal conductivity, and parameters of the capillary pressure and relative permeability functions) that are needed for predicting the flow of fluids and heat in fractured porous media; and (2) parameters of the petrophysical function that relates water saturation, porosity, and temperature to the dielectric constant.

ACCOMPLISHMENTS

We applied the approach to a large-scale *in situ* heater test that was conducted at Yucca Mountain, Nevada, to better understand the coupled thermal, hydrological, mechanical, and chemical processes that occur in the fractured rock mass around a geologic repository for high-level radioactive waste. We examined the sensitivity of the most relevant thermal-hydrological and petrophysical parameters to the time-lapse GPR data and thermal-hydrological data (temperature and water content) collected before and during the four-year heating phase of the test. To demonstrate the feasibility of the approach, and as a first step toward comprehensive inversion, we applied the approach to estimate the permeability of the rock matrix.

SIGNIFICANCE OF FINDINGS

Preliminary results indicate that estimation of thermal-hydrological and petrophysical parameters is possible through the combination of geophysical, hydrological, and thermal measurements. The large-scale heater test provides a unique data set to which our approach can be further applied and tested.

RELATED PUBLICATIONS

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Kowalsky, M., S. Finsterle, J. Peterson, S. Hubbard, Y. Rubin, E. Majer, A. Ward, and G. Gee, Estimation of field-scale soil hydraulic parameters and dielectric parameters through joint inversion of GPR and hydrological data. Water Resour. Res. 41, W11425, doi:10.1029/2005WR004237, 2005.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Mechanisms for Scale Dependence of the Effective Matrix Diffusion Coefficient

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RESEARCH OBJECTIVES

Matrix diffusion denotes the exchange of solute mass (through molecular diffusion) between fluid in fractures and fluid in the rock matrix. Owing to the orders-of-magnitude slower flow velocity in the matrix compared to that in fractures, matrix diffusion can significantly affect solute transport in fractured rock, and therefore is an important process for a variety of problems, including remediation of subsurface contamination and geological disposal of nuclear waste. The effective matrix diffusion coefficient is a key parameter for describing this matrix diffusion process. Our previous studies have indicated that the effective matrix diffusion coefficient values, obtained from a large number of field tracer tests, are enhanced in comparison with local values and increase with test scale. The major objective of this study is to investigate the physical mechanisms behind this scale dependence.

APPROACH

Numerical experiments were performed to evaluate the effects of flow-path geometry in a fracture network (Liu et al., 2007a). The focus of the experiments was on solute transport in flow paths having geometries consistent with percolation theories and characterized by local flow loops formed mainly by small-scale fractures. Values for effective transport parameters were obtained by matching breakthrough curves from numerical experiments with an analytical solution for solute transport along a single fracture. To investigate the effects of property heterogeneity on the rock matrix, we also derived analytical expressions for the effective matrix-diffusion coefficient for two idealized fracture-matrix systems: a single fracture system associated with rock matrix heterogeneity along the water flow direction in the fracture, and a multiple fracture system with rock-matrix heterogeneity among different fractures (Liu et al., 2007b). These analytical results allow for direct demonstrations of relationships between the scale dependence and spatial variability of the rock-matrix diffusive properties.

ACCOMPLISHMENTS

Our study indicates that the observed scale-dependence of the effective matrix diffusion coefficient results from a combination of flow-path-geometry effects and the heterogeneity of rock-matrix diffusive properties. Numerical experiment results show that the matrix diffusion process associated with local flow loops formed by small-scale (or high-level) fractures (which is mostly ignored in current modeling practices) seems to be an important mechanism in causing the observed scale dependence (Figure 1). Our analytical results further demonstrate that different-scale heterogeneities of the rock-matrix diffusive properties also contribute to this scale dependence.

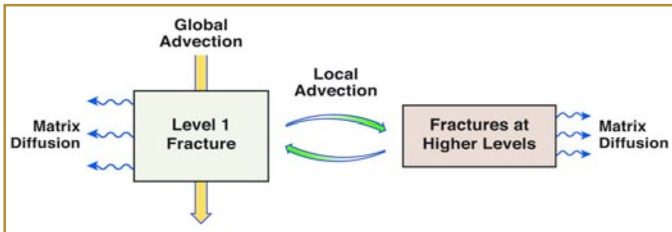

Figure 1. Effective matrix diffusion as a combination of local-scale advection and matrix diffusion in fractures at different scales.

SIGNIFICANCE OF FINDINGS

While the scale dependence of permeability and dispersivity has been an active research topic for many years, this study shows that the effective matrix diffusion coefficient, an important parameter controlling matrix diffusion processes, is also scale dependent. This finding has many important implications for problems involving matrix diffusion, including remediation of subsurface contamination in fractured rock and geological disposal of nuclear waste.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of the Chief Scientist, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Feedback of Coupled Thermal-Hydrological-Chemical Processes on Seepage at Yucca Mountain, Nevada: Role of Permeability and Capillarity Heterogeneity

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RESEARCH OBJECTIVES

In a recent publication (Mukhopadhyay et al., 2006), it was demonstrated that the coupled thermal-hydrological-chemical (THC) processes resulting from repository heating could alter the hydrological properties of the rock, which might in turn influence seepage into emplacement drifts. It was shown that seepage could occur when the THC processes were included in the predictive model, whereas none was predicted in the absence of these THC processes. These observations, however, were based on limited analysis: while heterogeneity in fracture permeability was included in the model, the corresponding heterogeneity in fracture capillarity (arising from the THC processes) was not accounted for. In this study, the influence of THC processes on seepage is investigated by accounting for heterogeneities in both fracture permeability and capillarity.

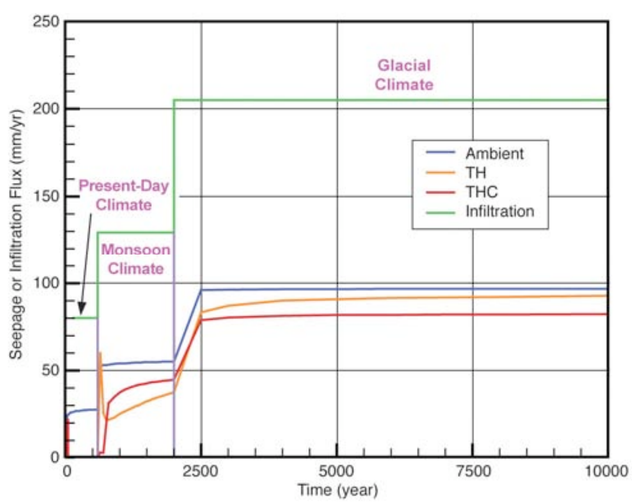

Figure 1. Comparison of ambient, TH, and THC seepage

APPROACH

A detailed description of the expected thermal-hydrological (TH) and THC processes in the unsaturated near-field fractured rock can be found elsewhere (Mukhopadhyay et al., 2006; Mukhopadhyay et al., 2007). In this study, TH and THC processes are simulated with the TOUGHREACT reactive transport numerical code. Ambient, TH, and THC simulations are performed in a two-dimensional vertical model domain extending from the ground surface to the water table. Heterogeneous fracture-permeability distributions are generated using measured air-permeability data from the host rock. Multiple realizations of the heterogeneous fracture permeability distribution are included in the simulations. Capillarity is allowed to change with changes in porosity and permeability, according to the Leverett scaling law. The fractured rock is modeled as two separate but interacting continua, one for the rock matrix and the other for the fractures.

ACCOMPLISHMENTS

No seepage was observed when the mean infiltration fluxes expected at Yucca Mountain were used in the simulations. Figure 1 shows the amount of seepage from ambient, TH, and THC simulations, when ten times the mean infiltration fluxes were used. After the thermal period is over, ambient seepage is predicted to be the largest and THC seepage the least. This observation is contrary to the findings of Mukhopadhyay et al. (2006); capillarity heterogeneity was ignored in that study, resulting in overprediction of local flow channeling and seepage.

SIGNIFICANCE OF FINDINGS

The observation that ambient seepage is larger than TH or THC seepage means that, for the prediction of repository performance, the seepage at all times, including the period when the temperature is elevated above ambient temperature, can be assumed to be ambient seepage. Further details can be found in Mukhopadhyay et al. (2007).

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02 –05CH11231.

Simple Model Representations of Transport in a Complex Fracture and Their Use in Long-Term Predictions

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RESEARCH OBJECTIVES

A complex fracture model for fluid flow and tracer transport was previously developed that incorporates all the important physical effects of a complex fracture zone. These effects include advection through a heterogeneous fracture plane, partitioning of flow into multiple subfractures in the third dimension, diffusion and sorption into fracture-filling gouge, small altered rock matrix blocks within the fracture zone, and the unaltered semi-infinite rock matrix on both sides of the fracture zone (Tsang and Doughty, 2003).

It is common, however, to represent the complex fracture by much simpler models consisting of a single fracture, without subfractures and with only the unaltered semi-infinite rock matrix for diffusion and sorption. The fracture may have a uniform (homogeneous) or heterogeneous transmissivity distribution over its plane, bounded on both sides by a homogeneous semi-infinite matrix. The parameters of the simple model can also be taken from laboratory data or calibration to short-term site-characterization (SC) data. The question posed by the present research is, how adequate are these simplified models for long-term performance assessment (PA) calculations that cover thousands of years?

APPROACH

We use a particle-tracking approach to calculate tracer transport in a complex fracture model, incorporating all the features described above, for a one-day SC tracer test and a 10,000-year PA prediction calculation. The results are considered the "real-world." Next, two simple fracture models, homogeneous and heterogeneous, are introduced. Properties for these simple models are taken either from laboratory data or found by calibration to one-day SC tracer-test breakthrough curves (BTC) obtained with the complex fracture model. Then, the simple models are used to simulate tracer transport at the PA time scale.

ACCOMPLISHMENTS

First, the results from laboratory-measured parameters are compared with those when data from the one-day SC tracer tests are used. The BTCs from the two cases are quite different, but by adjusting model properties, the simple models can reproduce peak arrival time and height. The overall match, however, is still poor (left frame of Figure 1).

Second, using simple models with SC-calibrated parameters for PA calculations causes order-of-magnitude errors in tracer BTCs: peak arrival time is 10 to 100 times too late and peak height is 100 to 1,000 times too small (right frame of Figure 1). On the other hand, using simple models with laboratory-measured properties of unfractured rock samples for PA calculations also produces erroneous results: peak arrivals and heights can be up to a factor of ten too early and high, respectively (right frame of figure). These are not general conclusions, since they depend on the parameter values assumed for the complex fracture model, and thus are more illustrative in nature, indicating the need for careful consideration.

SIGNIFICANCE OF FINDINGS

If a simple heterogeneous or homogeneous fracture model is used to predict tracer transport for a complex fracture at PA time scale, large errors may arise no matter what method is used to determine model properties. A remedy may be to determine properties by calibration to longer-term tracer tests (one to a few months rather than one to a few days), which will be sensitive to the detailed complex fracture features. A paper describing this work is in preparation.

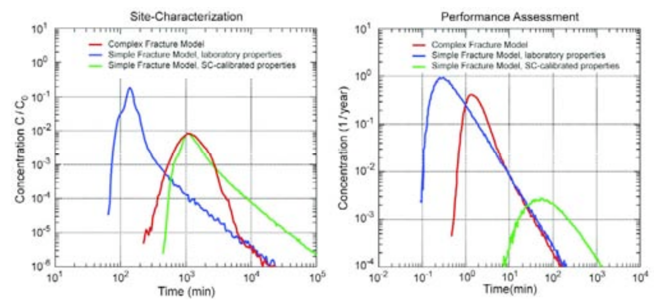

Figure 1. Tracer BTC for complex fracture model and simple fracture models with a single heterogeneous fracture. Left: short-term SC time scale. Right: long-term PA time scale.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

Work is supported by JAEA through a bi-national agreement between JAEA and the U.S. Department of Energy (DOE) and conducted under DOE Contract No. DE-AC02-05CH1123.

Estimating the Large-Scale Fracture Permeability of Unsaturated Rock Using Barometric Pressure Data

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RESEARCH OBJECTIVES

Fracture permeability is a key parameter for flow and transport simulations using dual-continuum approaches. However, how to properly estimate fracture permeability at large spatial scales is still a challenging task. The large-scale model parameters for fractures are in general more difficult to measure at the site than those for the rock matrix. The main objective of this study is to develop an approach for estimating large-scale fracture permeability, using the changes in subsurface pneumatic pressure in response to barometric pressure changes at the land surface.

APPROACH

Large-scale fracture permeabilities for the Yucca Mountain site are estimated through a comprehensive modeling effort by using pneumatic data measured from boreholes at the site. The modeling approach, built on a three-dimensional (3-D) mountain-scale unsaturated zone (UZ) flow model, incorporates pneumatic data into a modeling analysis of two-phase liquid and gas flow under ambient geothermal conditions. The gas-flow modeling studies are performed under present-day infiltration conditions using the site-specific geological model and characterization data. Calibration of model-predicted gas pressures against field-measured pneumatic data leads to a methodology for estimating fracture permeability in the unsaturated fractured rock.

ACCOMPLISHMENTS

A three-dimensional model of gas flow in the unsaturated fractured rock of Yucca Mountain has been developed. Large-scale fracture permeabilities of the site have been calculated through model calibration. This calibration was done through comparing gas-flow simulation results with the measured pneumatic data from underground boreholes. Fracture permeabilities, initially estimated by small-scale air-injection testing and 1-D model inversion, were adjusted to obtain an overall good match between the 3-D model predictions and pneumatic data (see Figure 1). The ability to match field pneumatic data observed from multiple sources, including pneumatic data over a long time, indicates the reliability of the numerical model in describing air and water flow processes within the Yucca Mountain UZ system, through better estimates of fracture flow properties.

SIGNIFICANCE OF FINDINGS

The results of this study indicate that using field-measured pneumatic data, in combination with numerical modeling analyses, provides a practical and powerful technique for estimating flow properties of vadose zone formations. Periodic responses of subsurface gas-pressure signals to surface barometric-pressure changes, which are easy to measure, may reveal invaluable information on gas mobility in unsaturated porous media. In addition, this work demonstrates that multidimensional effects on model-estimated permeability are significant when determining fracture permeability in heterogeneous fractured media. These effects can be captured only by 3-D modeling analyses on relevant model scales.

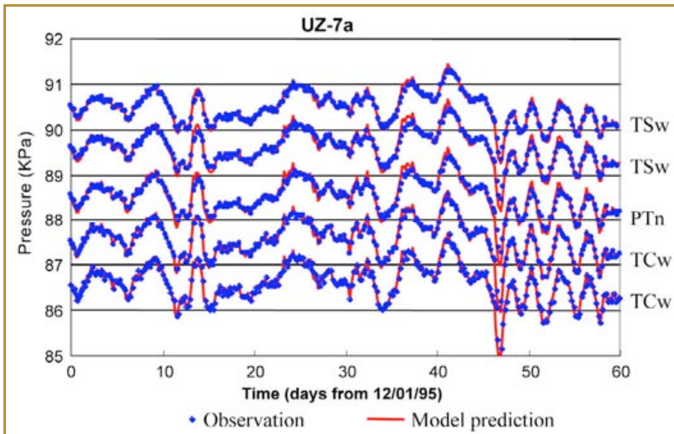

Figure 1. Comparison of simulated and observed gas pressures at borehole UZ-7a over a 60-day period, with 3-D model calibration.

RELATED PUBLICATIONS

Wu, Yu-Shu, Keni Zhang, and Hui-Hai Liu, Estimating large-scale fracture permeability of unsaturated rock using barometric pressure data. LBNL-57614. Vadose Zone Journal, 5, 1129–1142, 2006.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Investigation of Unsaturated Flow Patterns in Fractured Rock Using an Integrated Modeling Approach

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RESEARCH OBJECTIVES

Characterizing percolation patterns in unsaturated fractured rock poses a significant challenge to modeling investigations, because of the heterogeneous nature of unsaturated media and the many variables impacting unsaturated flow. The primary objective of this work is to quantitatively characterize percolation patterns in the fractured rock of the unsaturated zone (UZ) of Yucca Mountain, using an integrated modeling methodology.

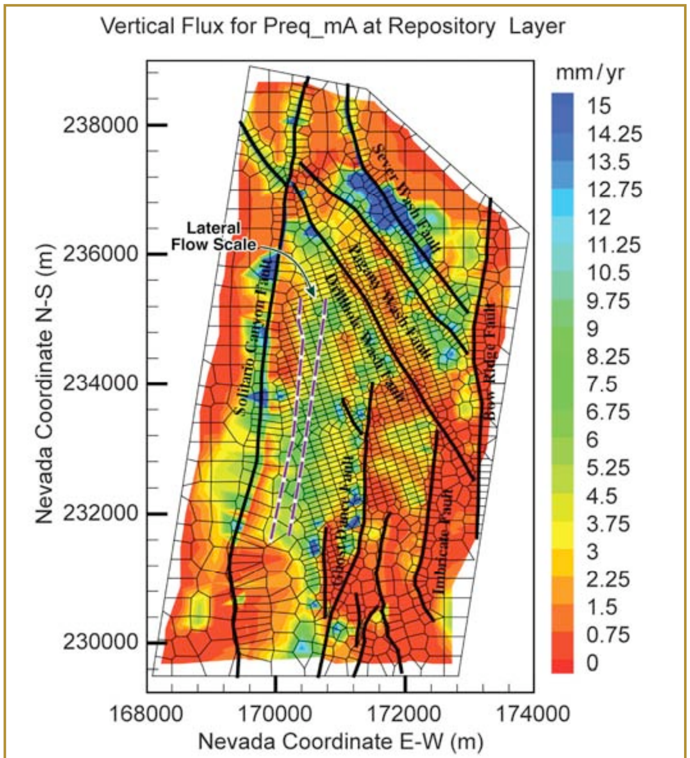

Figure 1. Simulated percolation fluxes at the repository horizon, using the present-day, mean infiltration scenario, base-case model results.

APPROACH

The integrated modeling approach combines a wide variety of field data into a comprehensive three-dimensional numerical model for flow pattern analyses. It takes into account the coupled processes of fluid and heat flow and chemical isotopic transport in Yucca Mountain's highly heterogeneous, unsaturated fractured tuffs. The fractured rocks are represented by a dual-permeability media. The main activities of study include (1) UZ model description; (2) model calibration using pneumatic, moisture, and geochemical data; (3) simulated percolation pattern analysis; and (4) assessment of percolation patterns and flow behavior using thermal and geochemical data.

ACCOMPLISHMENTS

An integrated modeling approach was used in a large-scale field study characterizing percolation patterns in the UZ of Yucca Mountain, The developed model integrated different field-observed data, such as moisture, gas pressure, chloride, and temperature data, into one single 3-D UZ flow and transport model. This combined model calibration provided a consistent cross-check or verification of model results, as well as better insight into UZ flow patterns. The integrated modeling effort also provided consistent model predictions for different but interrelated hydrological, pneumatic, geochemical, and geothermal processes. Most importantly, such an integrated approach improved the capability and credibility of numerical models in characterizing subsurface flow and transport processes.

The important findings from this study were: (1) at Yucca Mountain, water may not flow directly downward in a thick, heterogeneous unsaturated zone, but rather may be diverted laterally towards the east, along the sloping layers, and focused into major faults; and (2) lateral flow diversion occurs mainly at the Calico Hills formation (CHn), the stratigraphic unit below the repository horizon, resulting from the presence of perched water or thick low-permeability layers. Under the current hydrogeological conceptualization, faults act as major flow paths through the CHn or below the repository horizon. In addition, the modeled percolation fluxes show that fracture flow is dominant in the welded tuff, both at the repository horizon and at the water table, while the matrix carries the majority of water percolation through the nonwelded tuff. Figure 1 shows the simulated flux distribution at the repository horizon.

SIGNIFICANCE OF FINDINGS

The integrated modeling approach provides a practical modeling tool for characterizing flow and transport processes in complex subsurface systems and results in better understanding of percolation patterns and flow behavior through the Yucca Mountain UZ.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Coupling Seepage and Radionuclide Fate/Transport in and around Emplacement Drifts at Yucca Mountain

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RESEARCH OBJECTIVES

The objectives of this project are to: (1) develop a quantitative model of coupled thermal, hydrological, and chemical (THC) processes potentially leading to brine formation on top of waste packages and/or a drip shield and (2) dynamically integrate such a model into the larger-scale models of processes within and around waste emplacement tunnels, as well as into the smaller-scale waste-package corrosion models.

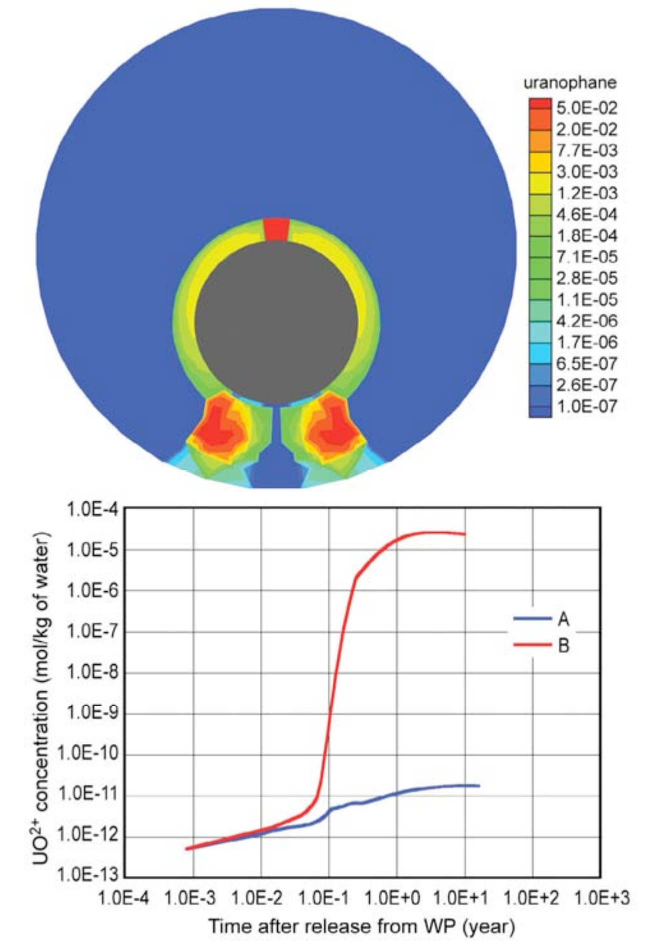

Figure 1. Simulated distribution of uranophane (mol/ m^3 of medium) precipitated after 25 years of continuous dripping (top) and simulated time evolution of UO_2^{+2} concentration at the base of the drift with (A) and without (B) consideration of uranophane precipitation.

APPROACH

Process models were implemented into TOUGHREACT to allow modeling of (1) evaporative concentration to very high ionic strength, (2) boiling point elevation due to dissolved salts, (3) boiling/evaporation to dryness, and (4) salt deliquescence. An integrated near-field/in-drift THC simulation was run using a vertical 2-D grid extending from near the ground surface to the groundwater table, and covering a width equal to half the design drift spacing of 81 m. The integrated model was then used to simulate a discrete dripping event within the drift. The model considered the release of radionuclides into seepage water as this water contacts the waste package and flows through the invert. The precipitation of uranophane and Np-uranophane was also considered. These minerals form in the invert from the neutralization of mildly acidic seepage water by clay minerals.

ACCOMPLISHMENTS

The main findings from this modeling effort are as follows: (1) the near-field and in-drift brine chemical evolution is dominated by the precipitation of NaCl, $CaSO_4$, and $CaCO_3$; (2) the generation of acid gases at high evaporative concentration yields P_{HCl} ~10^{-7} bar at boiling temperatures, with pH staying >5 in condensation areas; (3) the clay minerals in the invert neutralize the pH of seepage water, although this result is sensitive to assumptions regarding the kinetics of reactions with clays; (4) the drift invert may act as a pH buffer that promotes the precipitation of uranophane and impedes further downward migration of radionuclides at elevated concentrations (Figure 1). However, the pH buffer effect is subject to the content and composition of the clay minerals in the invert.

SIGNIFICANCE OF FINDINGS

The model captures some of the processes involved in salt formation and radionuclide transport, and can be further applied to capturing the details of radionuclide transport between the waste form and the rock through the invert.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of the Chief Scientist, of the U.S. Department of Energy (DOE) under DOE Contract No. DE-AC02-05CH11231.

Evaluation of Uncertainty in Infiltration Scenarios at Yucca Mountain, Nevada

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RESEARCH OBJECTIVES

An accurate estimate of infiltration rates is critical for the performance assessment of geological disposal of the high-level nuclear wastes at Yucca Mountain. The key components considered in the current infiltration model for Yucca Mountain include climate information, water transport and storage in the shallow zone, evapotranspiration, and surface runon and runoff. As a result of the uncertainty in the input parameters, 40 different infiltration maps were generated with the same probability of occurrence. However, the estimated infiltration maps are subject to some uncertainties due to the fact that the infiltration model was developed without consideration of subsurface data, such as temperature and chloride concentration measurements.

APPROACH

We developed an approach based on the generalized likelihood uncertainty estimate (GLUE) methodology (Beven and Binley, 1992). The GLUE procedure requires a definition of a likelihood measure to quantify how well each infiltration map reproduces the measured data. For each infiltration map, a process model is used to simulate water percolation, chloride transport, and heat transfer within the Yucca Mountain unsaturated zone. The simulation results are compared to the observed data to evaluate the likelihood function. A higher weighting factor is assigned to infiltration maps that more closely reproduce the data. Because of the inherent subjectivity in the choice of a likelihood function, the use of GLUE introduces a new type of uncertainty: the epistemic uncertainty in the analysis. To consider this uncertainty, we extended GLUE to use multiple likelihood measures and combine the results. The proposed likelihood functions cover a certain range of different functional types. The final weighting factor is an average of the weighting factors calculated from all the selected likelihood functions.

ACCOMPLISHMENTS

An effort was made in this study to handle the uncertainties in defining the likelihood function in the GLUE procedure. Specifically, four likelihood measures, each having a different evaluation focus and addressing a different aspect of model behavior, were chosen to assign weighting factors for the selected infiltration maps. Although the results from these likelihood functions varied, they consistently assign higher weights to the same infiltration maps. The final averaged weighting factors and their uncertainties were determined to weigh infiltration scenarios in the probabilistic performance assessment calculation.

SIGNIFICANCE OF FINDINGS

Net infiltration is a key hydrologic parameter for controlling percolation rate, groundwater recharge, potential seepage into waste emplacement drifts, and radionuclide transport—and therefore a key parameter in evaluating repository performance at Yucca Mountain. The GLUE method was developed to constrain the infiltration-rate uncertainties by using additional subsurface data collected from the unsaturated zone. Although the study is done for a specific setting, it provides a general framework from which to consider different types of uncertainty in environmental applications.

RELATED PUBLICATIONS

Beven, K., and A. Binley, The future of distributed models: Model calibration and uncertainty prediction. Hydrological Processes, 6, 279–298, 1992.

Wu, Y-S., et al., UZ Flow Models and Submodels, MDL-NBS-HS-000006, REV 03, June 2007.

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